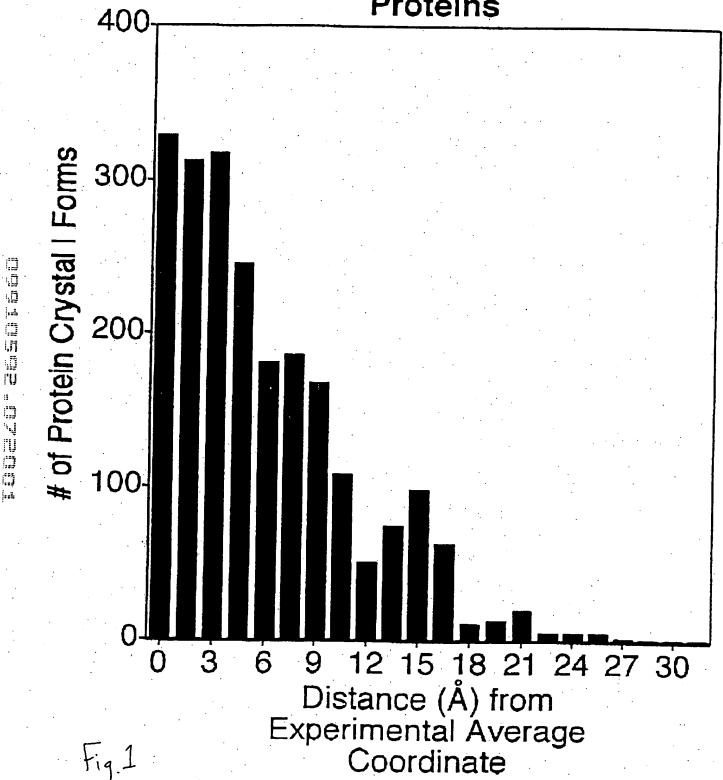
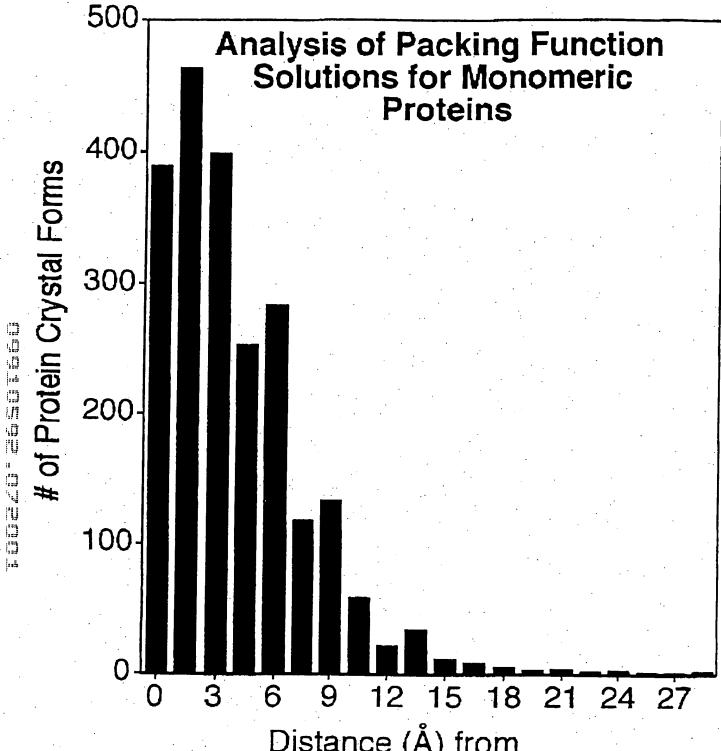
-- BRIEF DESCRIPTION OF THE DRAWINGS

- FIG. 1 shows a first protein crystal packing function histogram utilizing the method of the invention and based on providing the number of possible configurations for a given protein or other molecule of interest with a resolution in Angstroms.
- FIG. 2 shows a second protein crystal packing function histogram utilizing the method of the invention and based on providing the number of possible configurations for a given protein or other molecule of interest with a resolution in Angstroms.
- FIG. 3 shows a flow chart for the calculation routine of the current invention used to resolve the unphased diffraction amplitudes of the SHSB representations of the current invention.
- FIG. 4 shows a space filling schematic for a mathematical representation of the orthorhombic space group of the invention.
- FIG. 5 shows a flow chart for the calculation routine of the current invention used to resolve the unphased diffraction amplitudes of the SHSB representations into a Fourier Transformation of the model crystal of the molecule of interest utilizing a fractionalization matrix.
- FIG. 6 shows a representation of an Expanded Direct Space Basis Function of the invention.
- FIG. 7 shows a representation of a Component Direct Space Basis Function of the invention and the Component Fourier Transformations following there from. --

Analysis of Packing Function Solutions for Monomeric **Proteins**

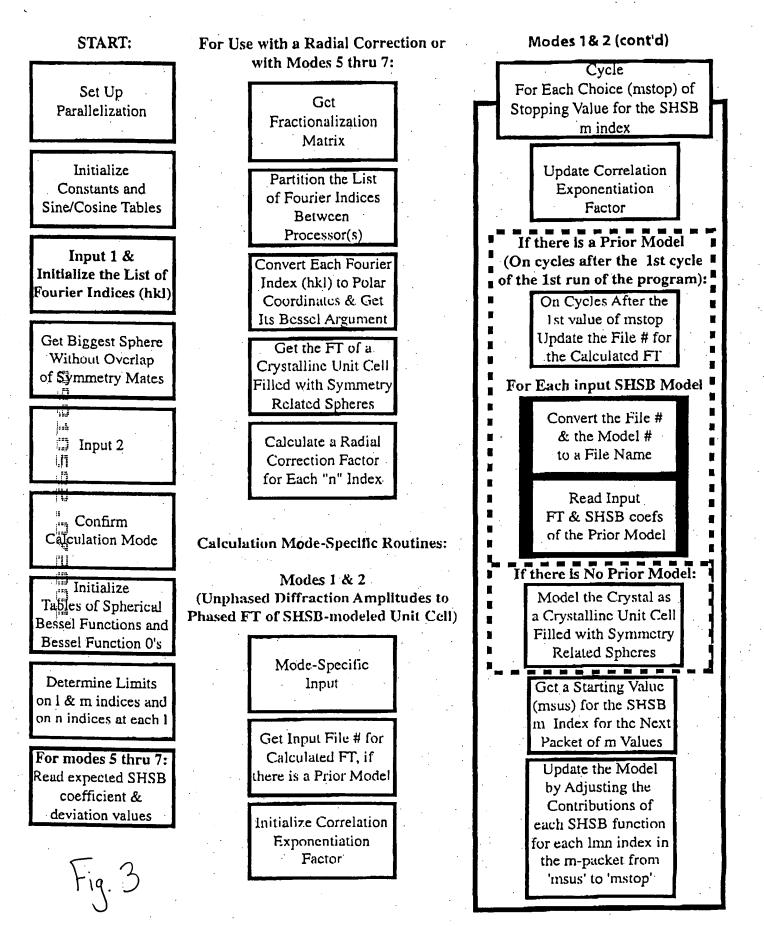


The state of the s



Distance (Å) from Experimental Average Coordinate

Fig. 2



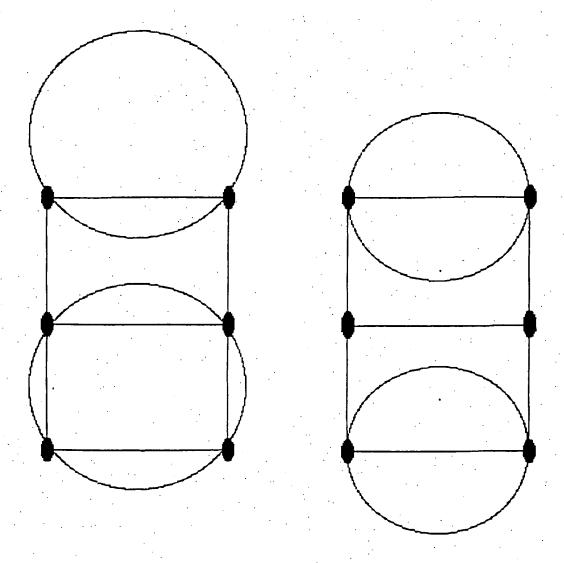


Figure A schematic example: Two choices for filling the same portion of a crystal unit cell from an orthorhombic Spacegroup. Although the spheres on the right are smaller than those on the left, for some crystals, the local maximum in the packing on the right wold be the packing of maximal consistency with the crystallographic data.

Figure 4.

Initialize Fractionalization Matrix

Initialize the Equal Partitioning of the Fourier (hkl) Index between Processors

On 1st Cycle of 1st Run:

Prescale Observed
Diffraction to that
of a Unit Cell of
Spheres

Define the First
SHSB Index Triplet
(Imn) for which to
Consider Model |F|'s

Irritialize for Indexby-Index Update of Origin-Centered SH\$B Basis Function

Modes 4 & 5 only: Intialize Buffers for Cumulative Update of

Foürier Representation

Initialize Pointers to Stored Fourier Representations of Model and of Basis

Mode 3 only:

Get File Name from File # & Open It to Let SHSB Coefs, be Read For each "m" Index (0 to maximum "m")

For Each hkl in this Partition:

Update "m" Recursion Formula for Fourier Representation of the Origin-Centered SHSB

For each "I" Index (present "m" to maximum "I")

For Each hkl in this Partition:

Update "I,m" Recursion Formula for Fourier Representation of the Origin-Centered SHSB

For each "n" Index (1 to maximum "n" for each "l")

For Each hkl in this Partition:

Update "n" Recursion Formula for Fourier Representation of the Origin-Centered SHSB

Depending on Mode:

Choose the # of Passes and # of Presumed Phase Angles Needed for the SHSB coef. with this SHSB index (Imn)

Set the Presumed Amplitude of the Origin-Centered SHSB Basis Function

FIRST PASS:

Initialize Registers:
Overall Comparison
of Correlation Coef.
& Other Statistics

Renitialize Pointers to Storage Sites for Fourier Representations of the Full-Unit-Cell SHSB Basis

Parallel Processor Version:

Set # of calculations to: (# of presumed values of SHSB coef.'s phase)

(# of stored accumulated SHSB models for trial combination with this new SHSB component)

Given: # of processors # of hkl partitions # of calculations Get: # of required rounds of trial combinations

For each round of trial combination on this processor

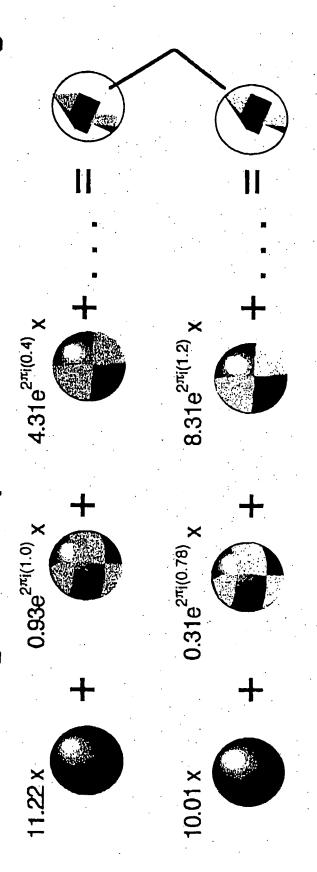
Single Processor Version: (Outer Loop)

For each presumed value of the SHSB coef. 's phase

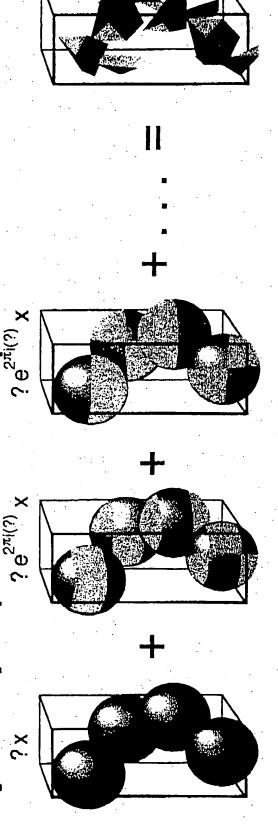
Initialize Registers: Angular Comparlson of Correlation Coef. & Other Statistics

Fig. 5

Identical Image from Expansions about Different Origins:

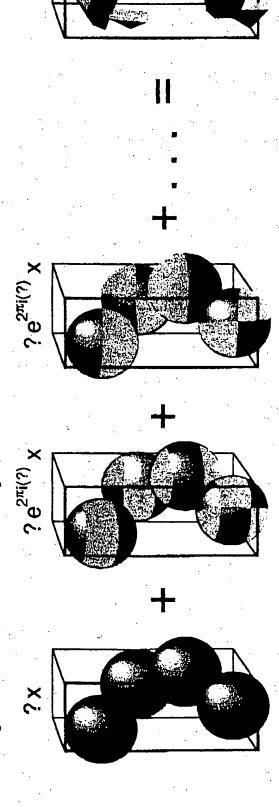


Symmetry Expanded Direct Space Basis Functions:



With a properly chosen origin, 45-55% of the unit cell can be expanded. (Most protein crystals are > 45% solvent.)

Component Direct Space Basis Functions:



Component Fourier Transforms:

$$a_{001}F_{solo}^{001}(hkl) + a_{211}F_{solo}^{211}(hkl) + a_{111}F_{solo}^{111}(hkl) + \dots = F_{obs}(hk)$$

$$a_{\infty_1} = \sum_{hkl} F^*_{solo}$$
 (hkl) F_{obs} (hkl) [presume $\phi = 0.00$ to start]

$$F_{\text{accum}}(hkl) = a_{001} F_{\text{solo}}^{001}(hkl)$$

$$a_{211} = \sum_{hkl} F_{solo}^* (hkl) (|F_{obs}(hkl)| - |F_{accum}(hkl)|) e^{2m \phi^n(hkl)}$$

$$F_{\text{accum}}^{\text{n+1}}(\text{hkl}) = F_{\text{accum}}^{\text{n}}(\text{hkl}) + a_{211}F_{\text{solo}}^{211}(\text{hkl})$$

15